CLIVAR Indian Ocean (I6S) 2008 Cruise Readme File

Class of Data: Surface ocean carbon dioxide concentrations

Dataset Identifier: Expo Code 33RR20080204

Statement of how to cite dataset:

CLIVAR I6S website: http://www.aoml.noaa.gov/ocd/gcc/clivari6s

These data are made freely available to the public and the Scientific community in the belief that their wide dissemination will lead to greater understanding and new scientific insights. The availability of these data does not constitute publication of the data. We rely on the ethics and integrity of the user to assure that the AOML ocean carbon group receives fair credit for our work. Please consult with us prior to use so we can insure that the quality and limitations of the data are accurately represented.

Cruise Information:

This cruise was part of the CLIVAR/CO2 repeat hydrography program (see http://ushydro.ucsd.edu/). The Scripps Institution of Oceanography's Research Vessel Roger Revelle departed Durban, South Africa on February 4, 2008 entering the southward-flowing Agulhas Current and traveled due south along a transect coinciding with Longitude 30 East into the Antartic Circumpolar Current down to the ice edge at 70 S returning to Cape Town, South Africa on March 16, 2008.

Scientist responsible for technical quality of dataset:

Rik Wanninkhof NOAA/AOML/Ocean Chemistry Division 4301 Rickenbacker Causeway Miami, Florida 33149 Rik.Wanninkhof@noaa.gov

Contact person for this dataset:

Esa Peltola NOAA/AOML/Ocean Chemistry Division 4301 Rickenbacker Causeway Miami, Florida 33149 Esa.Peltola@noaa.gov

Timestamp for initial submission of dataset: 4/27/08

Timestamp for the most recent update of dataset: 4/27/08

Timestamp period the dataset refers to: 2/05/2008 - 3/14/2008

Geographic area the dataset refers to:

List of variables included in this dataset:

COLUMN 1.	HEADER GROUP/SHIP:	EXPLANATION AOML_Revelle.
2.	CRUISE_DESIGNATION:	IO6S(2008)_33RR20080204
3.	JD_GMT:	Decimal year day.
4.	DATE_DDMMYYYY:	The date format has been changed from previous files to conform with the IOCCP recommendations.
5.	TIME_HH:MM:SS:	GMT time. Local time = GMT time + 2 hours.
6.	LAT_DEC_DEGREE:	Latitude in decimal degrees (negative values are in the southern hemisphere).
7.	LONG_DEC_DEGREE:	Longitude in decimal degrees (negative values are in the western hemisphere).
8.	xCO2W_PPM:	Mole fraction of CO2 (dry) in the headspace equilibrator at equilibrator temperature (Teq) in parts per million.
9.	xCO2A_PPM:	Mole fraction of CO2 in air in parts per million.
10.	PRES_EQUIL_hPa:	<pre>Barometric pressure in the lab in hectopascals(1 hectopascal = 1 millibar).</pre>
11.	PRES_SEALEVEL_hPa:	Barometric pressure from ship's barometer, corrected to sea level in hectopascals (1 hectopascal = 1 millibar).
12.	EQTEMP_C:	Temperature in equilibrator water in degrees centigrade. Temperature in equilibrator measured with a calibrated thermistor.
13.	SST(TSG)_C:	Temperature from the ship's thermosalinograph in degrees centigrade.
14.	SAL(TSG)_PERMIL:	Salinity from the ship's thermosalinograph on the Practical Salinity Scale.
15.	WATER_FLOW_L/MIN:	Water flow through equilibrator in liters per minute.
16.	GASFLOW_IR_ML/MIN:	Gas flow through the Licor infrared analyzer before the flow is stopped in milliliters per

minute.

17.	TEMP_IR_C:	Temperature of the Licor infrared analyzer sample cell in degrees centigrade.
18.	PRES_IR_hPa:	Pressure in the Licor infrared analyzer in hectopascals. NOTE: There is no pressure sensor in the Licor but since it is vented to atmosphere prior to measurement, this value is the same as the pressure in the lab (number 10 above). (1 hectopascal = 1 millibar).
19.		GREE: Ship's heading from ship's navigation system in degrees with $0 = North$ and $90 = East$.
20.	SHIP_SPEED_KNOT:	Ship's speed from ship's navigation system in knots.
21.	WIND_DIR_REL_DEGREE:	Wind direction relative to the ship from ship's navigation system in degrees with $0 = \text{from the bow and } 90 = \text{from starboard.}$
22.	WIND_SPEED_REL_M/S:	Wind speed relative to the ship from ship's navigation system in meters per second.
23.	fCO2W@SST_uATM:	Fugacity of CO2 in sea water in microatmospheres.
24.	QC_FLAG_WATER:	Quality control flag for sea water $xCO2$ and $fCO2$ values with $2 = good$ value, $3 = questionable$ value, $4 = bad$ value, and $9 = no$ measurement taken.
25.	fCO2a_uATM:	Fugacity of CO2 in air in microatmospheres.
26.	QC_FLAG_AIR:	Quality control flag for air $xCO2$ and $fCO2$ with 2 = good value, 3 = questionable value, 4 = bad value, and 9 = no measurement taken.
27.	dfCO2_uATM:	Sea water fCO2 - air fCO2 in microatmospheres. This uses the average air value for the current hour.
28.	FLUORO_uG/L:	Reading from the fluorometer in micrograms per liter. There is no fluorometer data for this cruise.
29.	WIND_SPEED_TRUE_M/S:	True wind speed in meters per second.
30.	WIND_DIR_TRUE_DEGREE	: True wind direction in degrees were 0 = North and 90 = East.

31. AIR_TEMP_C: Outside air temperature from ship's computer system in degrees centigrade.

The following fields have been QC'ed by the CO2 group:

GROUP SHIP CRUISE JD GMT DATE DDMMYYYY TIME HH:MM:SS LAT DEC DEGREE LONG DEC DEGREE xCO2W PPM xCO2A PPM PRES EQUIL hPa EQTEMP C WATER FLOW L/MIN GASFLOW IR ML/MIN TEMP IR C PRES IR hPa fCO2W@SST uATM QC FLAG WATER

The following fields are from the ship's onboard systems and the quality of this data cannot be verified:

PRES_SEALEVEL_hPa
SST(TSG)_C
SAL(TSG)_PERMIL
SHIP_HEADING_TRUE_DEGREE
SHIP_SPEED_KNOT
WIND_DIR_REL_DEGREE
WIND_SPEED_REL_M/S
FLUORO_UG/L
WIND_SPEED_TRUE_M/S
WIND_DIR_TRUE_DEGREE
AIR_TEMP_C

CO2 ANALYTICAL SYSTEM:

The concentration of carbon dioxide (CO2) in surface ocean water is determined by measuring the concentration of CO2 in gas that is in contact with the water. Surface water is pumped from an inlet in the ship's bow to the equilibration chamber. The chamber contains a water spray head, an enclosed gaseous headspace (~ 850 ml), and a pool of seawater (~ 750 ml) that continuously overflows to a drain. As the water flows through the chamber, the dissolved gases (like CO2) partition between the water and the headspace. At equilibrium, the ratio of CO2 in the water and in the headspace is influenced most by temperature, and that relationship is known. By measuring the concentration of CO2 in the headspace and the temperature in the chamber, the partial pressure (or fugacity) of CO2 in the surface water can be calculated.

CALCULATIONS:

The mixing ratios of ambient air and equilibrated headspace air are calculated by fitting a second-order polynomial through the hourly averaged response of the detector versus mixing ratios of the standards. Mixing ratios of dried equilibrated headspace and air are converted to fugacity of CO2 in surface seawater and water saturated air in order to determine the fCO2. For ambient air and equilibrator headspace the fCO2a, or fCO2eq is calculated assuming 100% water vapor content:

fCO2a/eq = xCO2a/eq (P-pH2O) exp (B11+2d12) P/RT

where fCO2a/eq is the fugacity in ambient air or equilibrator, pH2O is the water vapor pressure at the sea surface temperature, P is the atmospheric pressure (in atm), T is the SST or equilibrator temperature (in K) and R is the ideal gas constant (82.057 cm 3 -atm·deg $^-1$ ·mol $^-1$). The exponential term is the fugacity correction where B11 is the second virial coefficient of pure CO2

B11 = $-1636.75 + 12.0408T - 0.032795T^2 + 3.16528E - 5 T^3$ and d12 = 57.7 - 0.118 T

is the correction for an air-CO2 mixture in units of $cm^3 \cdot mol^{-1}$ (Weiss, 1974).

The calculation for the fugacity at SST involves a temperature correction term for the increase of fCO2 due to heating of the water from passing through the pump and through 5 cm ID PVC tubing within the ship. The water in the equilibrator is typically 0.2 $^{\circ}$ C warmer than sea surface temperature. The empirical temperature correction from equilibrator temperature to SST is outlined in Takahashi et al (1993):

fCO2w = fCO2eq Exp(0.0423 (SST-Teq))

INSTRUMENT DESIGN:

The general principle of instrumental design can be found in Wanninkhof and Thoning (1993), Ho et al. (1995), and Feely et al. (1998). The analyses are done with an infrared analyzer calibrated with three standard gases spanning the anticipated range of water and air values. The standard gases come from NOAA/CMDL in Boulder and are directly traceable to the WMO scale.

The standards used on the cruise are:

STANDARD	TANK #	CONCENTRATION	VENDOR
STD1	CA06827	284.71	CMDL
STD2	CA05334	380.98	CMDL
STD3	CA06380	448.29	CMDL

Salinity, SST, wind direction (both absolute and relative), wind speed (both absolute and relative), ship speed, ship course, sealevel pressure, air temp, latitude and longitude data are from the

ship's MET system log files.

Sampling Cycle:

The system runs on an hourly cycle during which 3 standard gases, 3 air samples from the bow tower and 8 surface water samples (from the equilibrator head space) are analyzed on the following schedule:

Mins. after hour	Sample
===========	=====
3.5	Low Standard
7.5	Mid Standard
11.5	High Standard
16.24	Water
20.5	Water
25.2	Water
29.5	Water
33.5	Air
37.5	Air
41.5	Air
46.2	Water
50.5	Water
55.2	Water
59.5	Water

Units:

All xCO2 values are reported in parts per million (ppm) and fCO2 values are reported in microatmospheres (uatm) assuming 100 % humidity at the equilibrator temperature for fCO2w and for SST at fCO2a.

Estimated overall uncertainty of measurement:

The xCO2eq measurements are believed accurate to 1 ppm. The fCO2@SST measurements are believed to be precise to 2 ppm.

Bibliography:

- DOE (1994). Handbook of methods for the analysis of the various parameters of the carbon dioxide system in sea water; version 2. DOE.
- Feely, R. A., R. Wanninkhof, H. B. Milburn, C. E. Cosca, M. Stapp and P. P. Murphy (1998). A new automated underway system for making high precision pCO2 measurements onboard research ships. Analytica Chim. Acta 377: 185-191.
- Ho, D. T., R. Wanninkhof, J. Masters, R. A. Feely and C. E. Cosca (1997). Measurement of underway fCO2 in the Eastern Equatorial Pacific on NOAA ships BALDRIGE and DISCOVERER, NOAA data report ERL AOML-30, 52 pp., NTIS Springfield.
- Wanninkhof, R. and K. Thoning (1993). Measurement of fugacity of CO2 in Surface water using continuous and discrete sampling methods. Mar. Chem. 44(2-4): 189-205.
- Weiss, R. F. (1970). The solubility of nitrogen, oxygen and argon in water and seawater. Deep-Sea Research 17: 721-735.
- Weiss, R. F. (1974). Carbon dioxide in water and seawater: the solubility of a non-ideal gas. Mar. Chem. 2: 203-215.
- Takahashi, T., J. Olafsson, J. G. Goddard, D. W. Chipman, and S. C. Sutherland (1993). Seasonal variation of CO2 and nutrients in the high-latitude surface oceans: a comparative study, Global Biogeochem. Cycles, 7, 843-878.

DATA QC:

The data for the following year days (JD) were initialized to -999.99 due to low water flow:

JD 29.996 29.996 30.002 30.002 30.002 30.035

30.036 32.756 32.756

The data for the following year days (JD) were removed due to low gas

JD 74.044 74.047 74.050 74.053 74.056 74.059 74.062 74.065 74.068 74.071 74.074 74.077 74.080 74.083 74.086

74.101 74.104 74.107 74.110 74.112 74.116 74.119

74.089 74.092 74.095 74.098

74.122 74.125 74.128 74.130

74.133 74.136

74.139 74.143 74.146

74.149

74.151

74.154

74.157

74.160

74.163

74.167

74.169

74.172

74.172

74.175

74.178 74.181

74.184

74.187

74.190

74.100

74.193 74.196

74.199

74.202

74.205

74.208

74.211

74.214

74.217

74.220 74.223

74.226

74.229

74.232

74.235

74.237

74.241

74.244

74.247

74.250

74.253

74.255

74.258

74.261 74.264

74.264

74.271

74.274

74.276

74.279

74.282

74.285

74.288

74.292 74.294

74.297

74.300

74.303

74.306

The salinity data for the following year days (JD) were removed (initialized to -999.99): JD 43.309 to JD.375.

The questionable fCO2a data for the following year days (JD) were removed due to stack gas contamination: JD 36.357 to JD 37.083, JD 38.761 to JD 38.875, JD 38.970 to JD 39.125, JD 43.428 to JD 43.458, JD 61.095 to JD 61.167, and JD 65.470 to JD 65.500.

There was a problem with the SST (SCS temperature) from JD 40.4166 to JD 43.3777. The SST data for this time interval was estimated in the following manner: The average difference between Tequil and SST for 100 points immediately before and after the data dropout was determined. This difference was subtracted from the Tequil to create a SST. The correction (the average difference of the Tequil and SST) was 0.17319 C.

There was a problem with the sealevel pressure from JD 35 to JD 45. A correction (the average difference between the equilibrator pressure and the sealevel pressure) was applied to the sealevel pressure utilizing the equilibrator pressure in the same manner as described above for SST. In this time interval, the sealevel pressure was determined assuming sealevel pressure = equilibrator pressure - 1.102 MB.

The following SST and Equilibrator temperature values were interpolated using the values immediately preceding and following the data dropout:

45.244

48.362

54.360

73.354

The following Equilibrator temperature values were interpolated using the values immediately preceding and following the data dropout:

50.818

51.559

52.538

54.362

56.297

59.982

63.056

63.059

The following Salinity values were interpolated using the values immediately preceding and following the data dropout:

58.198

59.089

59.086

67.273

The following SST values were interpolated using the values Immediately preceding and following the data dropout:

45.244

48.362

49.026

50.285

54.359

56.024

56.681

57.294

57.595

57.896

58.514

58.803

59.086

59.341

60.589

60.717

60.660

61.029

61.274

61.735

66.577 66.785

67.047

73.354